RVB-Gutzwiller approach

to strongly correlated superconductors

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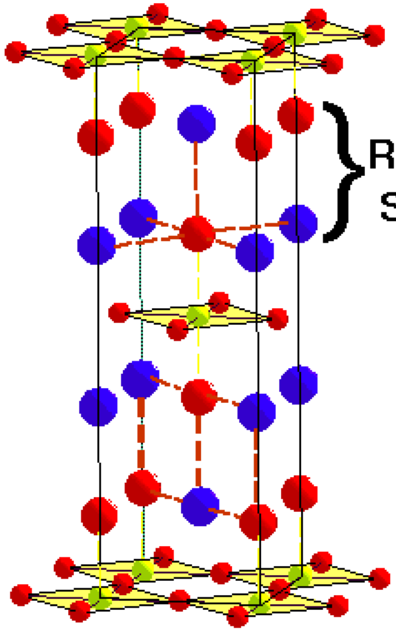
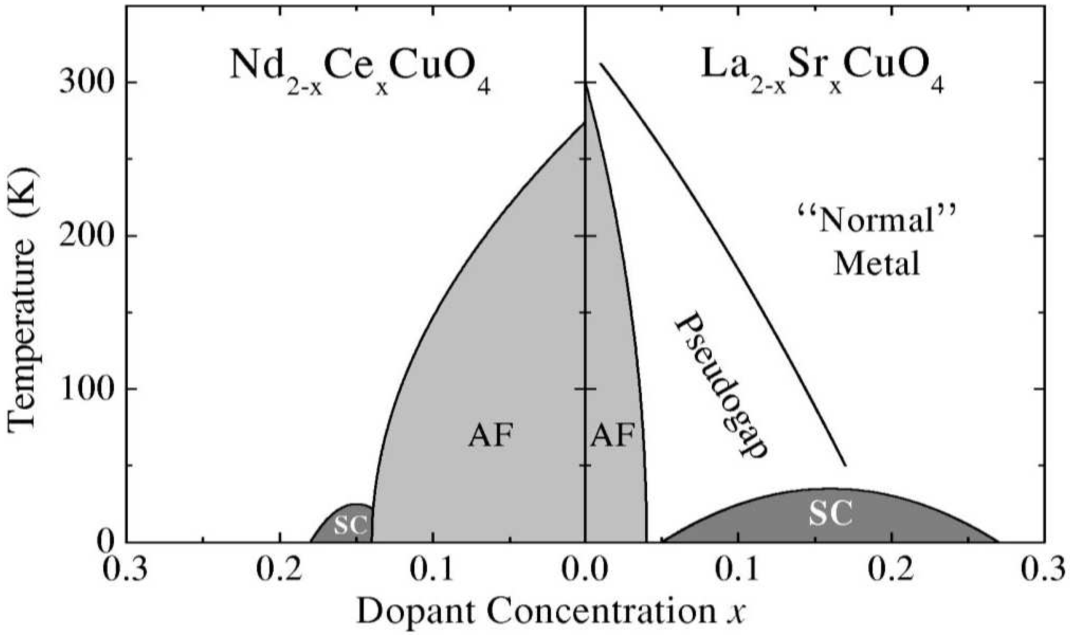
high-temperature superconductors





novelty

superconductivity in a doped oxide (bad metal)

doped Mott-Hubbard insulator

$T_c < T < T^*$ pseudogap phase: preformed pairs

BCS superconductivity

Bardeen-Cooper-Schrieffer

- BCS wavefunction

$$|\Psi_{BCS}\rangle = \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|0\rangle \qquad u_k^2/v_k^2 = \frac{1}{2}\left(1 \pm \frac{\xi_k}{\sqrt{\xi_k^2+\Delta_k^2}}\right)$$

- one-particle dispersion $\xi_k = \frac{\hbar^2 k^2}{2m} - \mu$
- Bogoliubov quasiparticles : $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$
- gap function Δ_k :

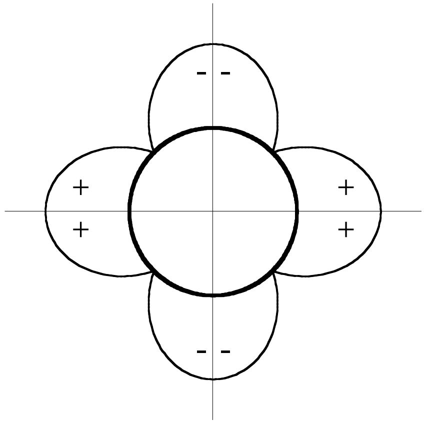
s-wave	Δ
d-wave	$\cos(k_x) - \cos(k_y)$

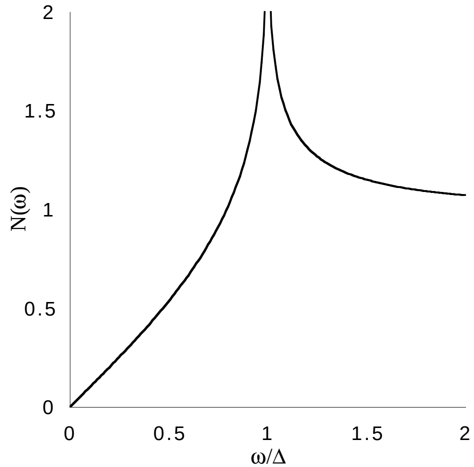
d-wave superconductivity

gap-function

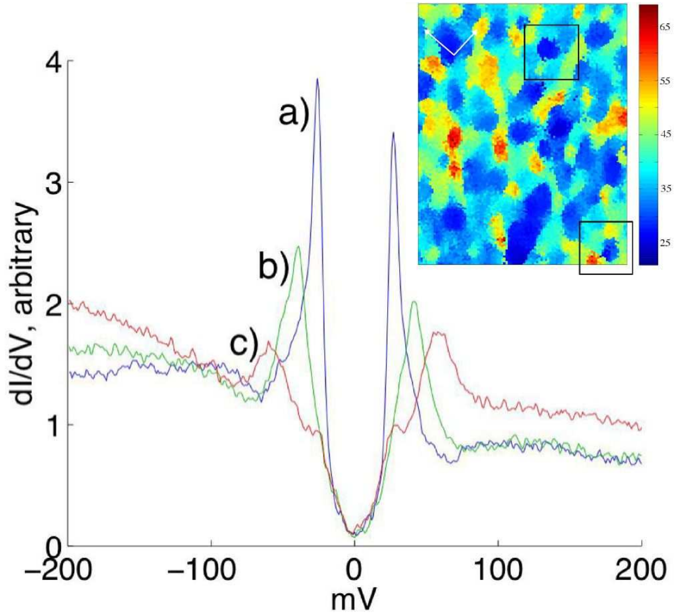
$$\Delta_k = \Delta(\cos k_x - \cos k_y)$$

▷ nodes along $(1,1)$ direction





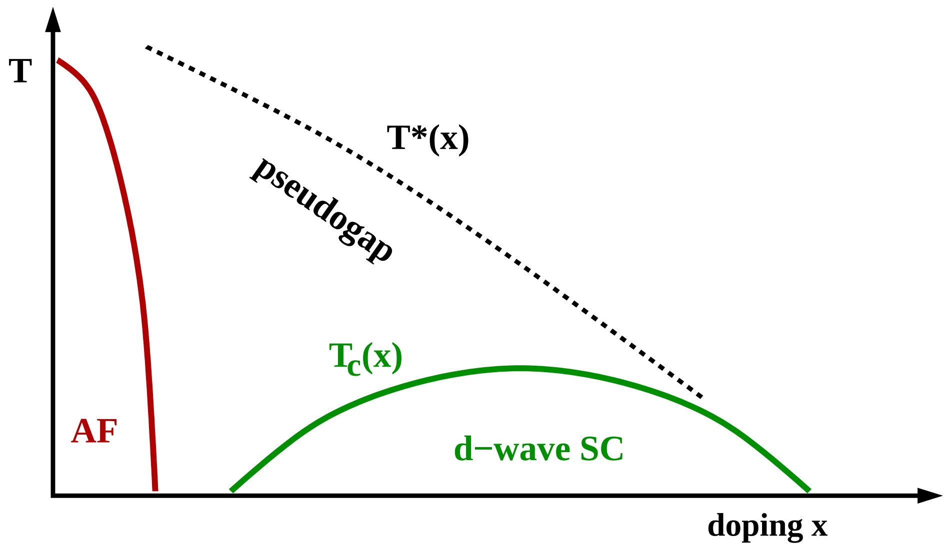
[Fang *et al.* '05]

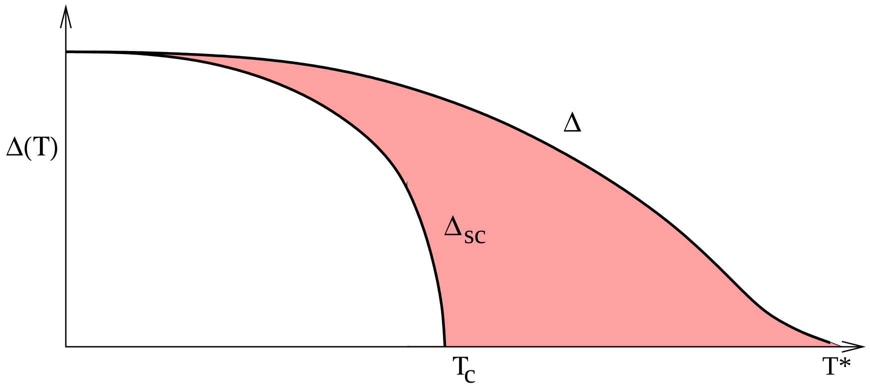


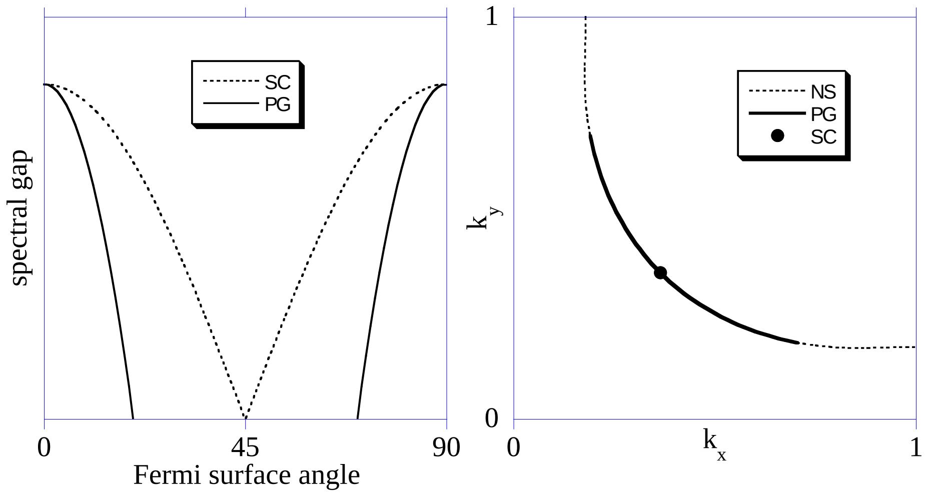
- predicted by theory
  - ▷ correlation-induced superconductivity
- experimental verification
  - ▷ phase-sensitive interference
  - ▷ tunneling, ARPES

central physical question: the pseudogap phase

What happens for $T > T_c$?







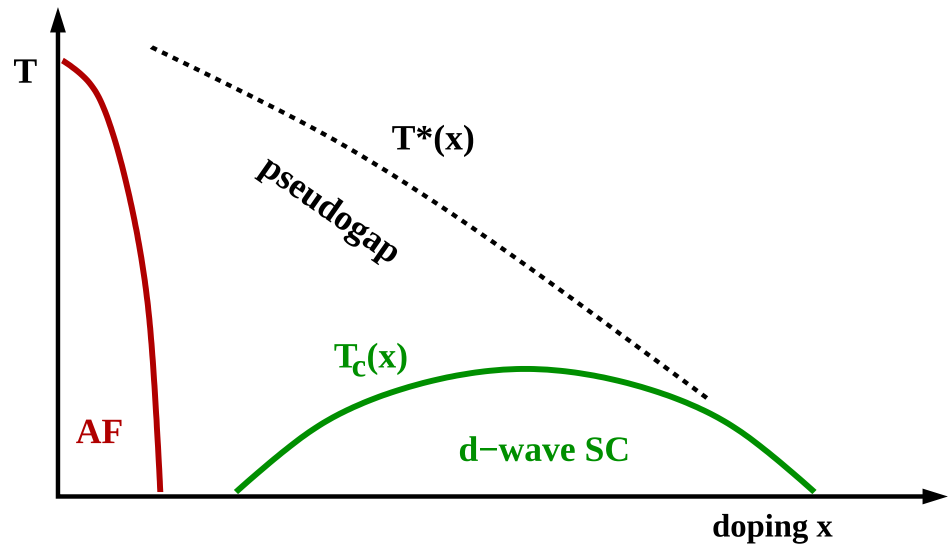
- one-particle excitations
  - ▷ transport, ARPES
  - ▷ pseudo $\Delta_k \approx \Delta(\cos k_x - \cos k_y)$

[Norman *et al* ‘98]

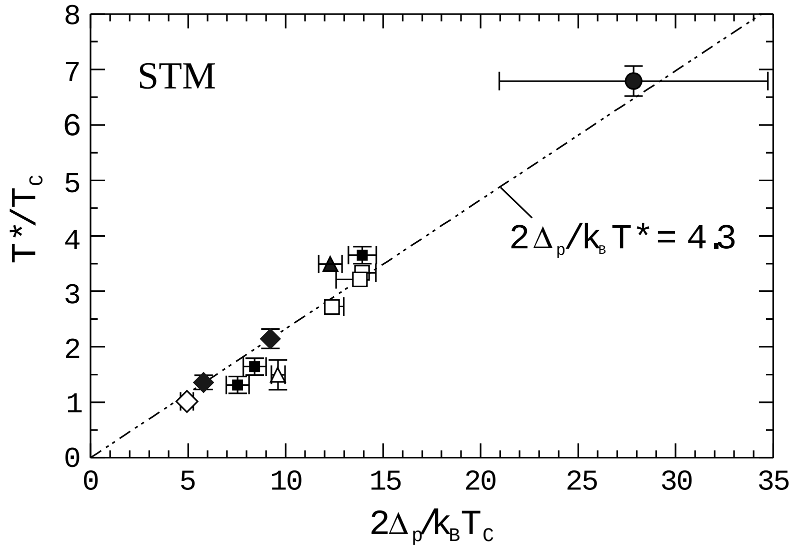
BCS ratio and preformed pairs

- universal for weak-coupling

$$\frac{2\Delta}{k_B T_c} = \begin{cases} 3.52 & \text{s-wave} \\ 4.3 & \text{d-wave} \end{cases}$$



[Kugler, Fischer, Renner, Ono, Ando ‘01]



- high-temperature superconductors :

$$\frac{2\Delta}{k_B T^*} = 4.3$$

doped Mott-Hubbard insulators

$$H = -t \sum_{<i,j>,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

strong correlation

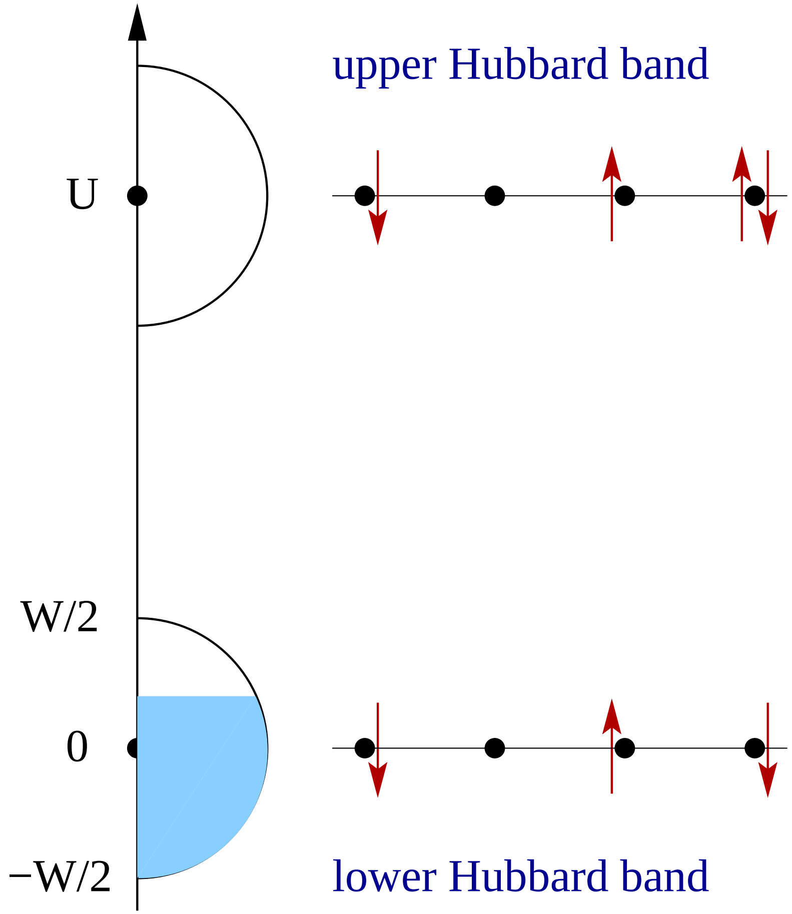
$U \gg t$: reduced double occupancy

$c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} |0\rangle$ has energy U

low-energy states

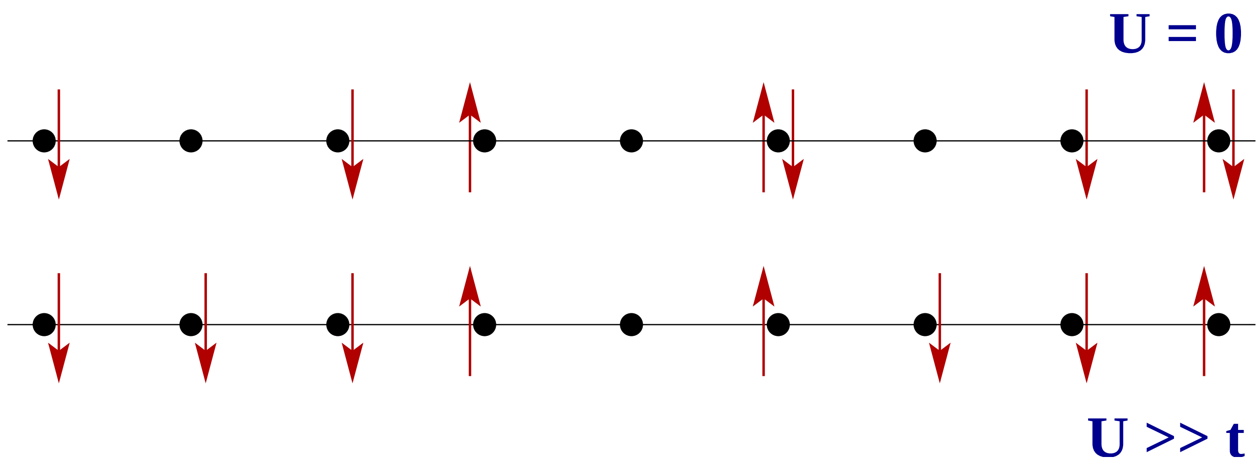
$c^\dagger_{i\sigma}|0\rangle$ singly-occupied

$|0\rangle$ empty sites



Mottness and enhanced phase fluctuations

reduction of particle number fluctuations by strong correlations



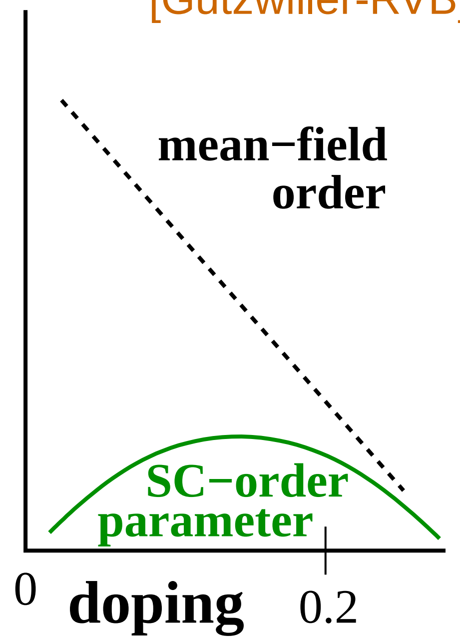
canonical conjugate variables $\langle \Delta N \rangle \langle \Delta \varphi \rangle \approx 1$

phase φ

particle number N

$$\left(\lim_{U/t \to \infty} \lim_{n \to 1} \langle \Delta N \rangle \to 0 \right) \iff \left(\lim_{U/t \to \infty} \lim_{n \to 1} \langle T_c \rangle \to 0 \right)$$

[Gutzwiller-RVB]



- Mottness results in diverging phase fluctuations

nodal Fermi velocity

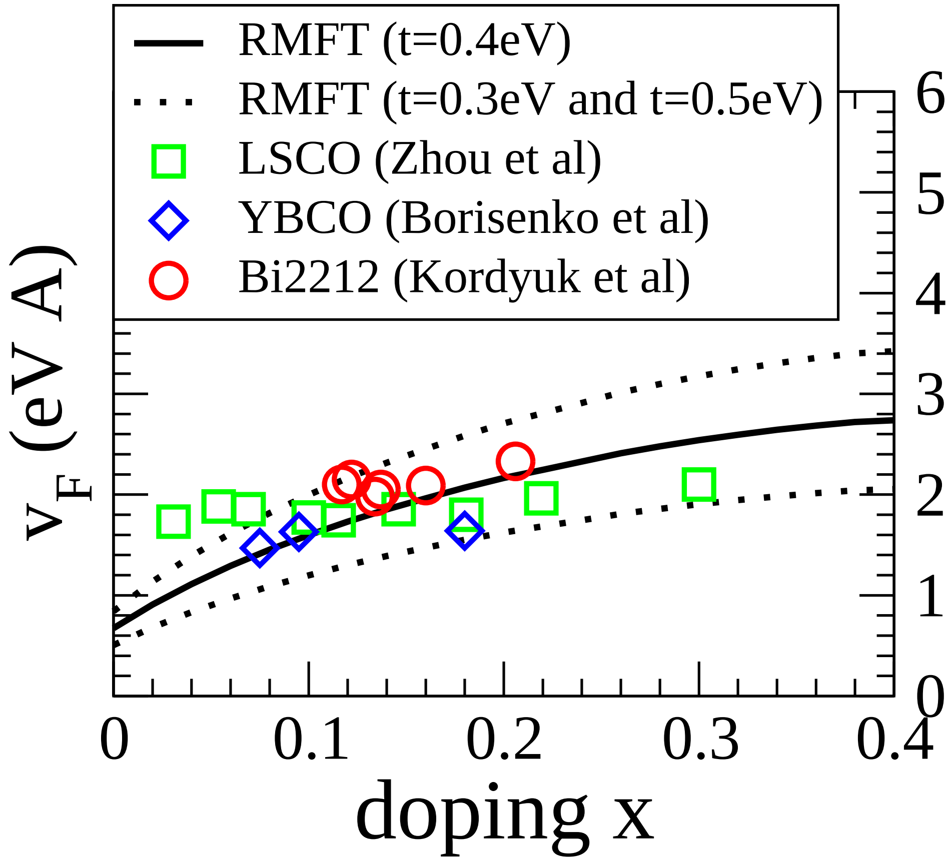
- nodes along $(1,1)$ direction

$$v_F = \frac{d\varepsilon(k)}{dk}$$

- RVB-Gutzwiller

$$\lim_{U/t\to\infty}\lim_{n\to 1} v_F \propto J = 4\frac{t^2}{U}$$

[Edegger, Muthukumar, Gros, Anderson '06]



experiment & theory

$$\lim_{U/t\to\infty}\lim_{n\to 1} v_F \to \text{const}$$

nodal quasiparticle weight renormalization

one particle Greens function

$$G(k,\omega) = \frac{1}{\omega - \xi_k - \Sigma(k,\omega)} \approx \frac{Z}{\omega - v_F(k-k_F) + i\delta_k} + G_{inc}(k,\omega)$$

- quasiparticle weight

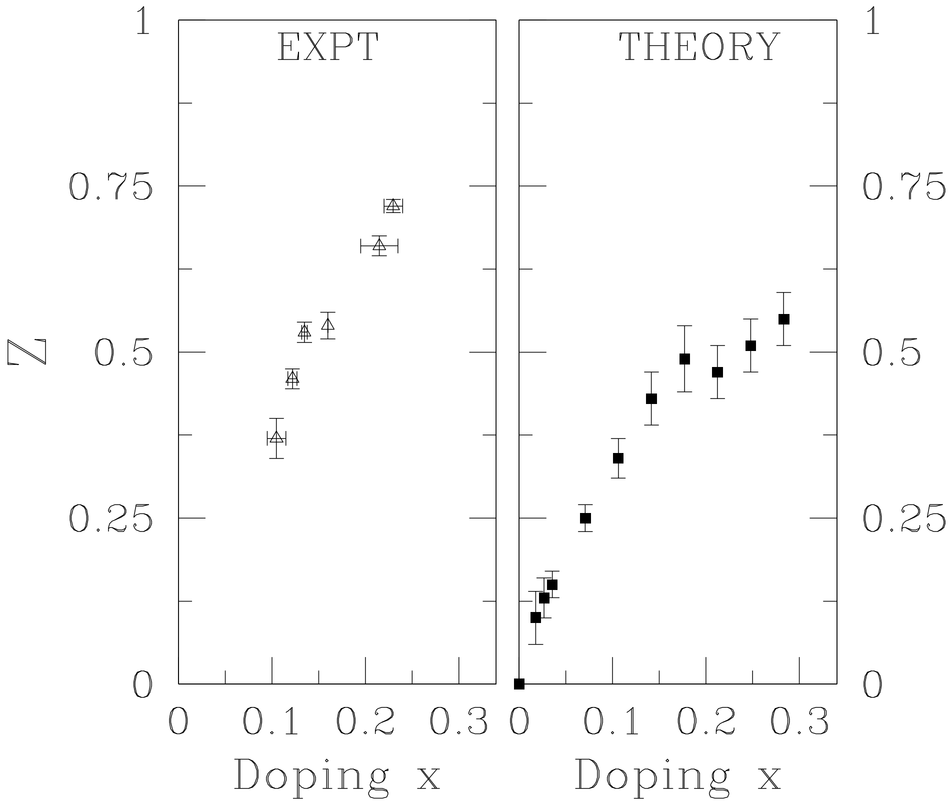
[Johnson *et al.* '01]

[Randeria, Paramekanti, Trivedi '04]

$$Z = \frac{1}{1 - \partial Re\Sigma/\partial\omega}$$

- Fermi velocity

$$v_F = Z\left(v_F^0 + \frac{\partial Re\Sigma}{\partial k}\right)$$



theory & experiment(?)

$$\lim_{U/t\to\infty} \lim_{n\to 1} Z \to 0$$

diverging momentum dependence of self energy

theory & experiment

$$\lim_{U/t\to\infty}\lim_{n\to 1} v_F \longrightarrow \text{const}$$

$$\lim_{U/t\to\infty}\lim_{n\to 1} Z \longrightarrow 0$$

- Fermi velocity

$$v_F = Z\left(v_F^0 + \frac{\partial Re\Sigma}{\partial k}\right)$$

singular momentum dependence (nodal)

$$\lim_{U/t\to\infty}\lim_{n\to 1} \frac{\partial Re\Sigma}{\partial k} \propto \frac{1}{x} \longrightarrow \infty$$

- doping $x = 1 - n$

d-wave superconductivity in the Hubbard model

.. as predicted by strong coupling theories in the late eighties

[Gros; Kotliar & Liu; Ogata & Shiba; Zhang, Gros, Rice & Shiba, ..]

induced by antiferromagnetic exchange $\sim J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j$

.. not explicitly present in the original Hubbard model $J = 4t^2/U$

approaches

- numerical simulations

[Maier, Jarrell & Scalapino; Kotliar , ..]

- small-U RG

[Honerkamp, Salmhofer, Furukawa & Rice; Halboth & Metzner , ..]

- large-U canonical transformation

$$H_{t-J} = e^{iS} H e^{-iS} \approx -t \sum_{<i,j>,\sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j + \dots$$

Gutzwiller approximation

projected wavefunctions

$$|\Psi\rangle = P\,|\Psi_0\rangle = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})\,|\Psi_0\rangle$$

projected Hilbert space : $|\Psi\rangle$

pre-projected Hilbert space : $|\Psi_0\rangle$

renormalization scheme

$$\frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \approx g\,\frac{\langle\Psi_0|\hat{O}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \qquad g_t = \frac{1-n}{1-n/2}$$

renormalization factors

Hilbert space counting arguments

renormalization scheme

un-projected Hilbert space	Hubbard Hamiltonian
$\Downarrow$ canonical transformation $e^{iS} H e^{-iS}$	$\Downarrow$
projected Hilbert space	t-J Hamiltonian
$\Downarrow$ Gutzwiller renormalization g	$\Downarrow$
pre-projected Hilbert space	renormalized Hamiltonian

$$\frac{\langle\Psi|H_{t-J}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \approx \frac{\langle\Psi_0|H_{t-J}^{(renor)}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

$$H_{t-J}^{(renor)} = g_t T_e + g_s J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$g_t = \frac{1-n}{1-n/2}, \qquad g_s = \frac{1}{(1-n/2)^2}$$

renormalized molecular-field theory

pre-projected Hilbert-space

$|0\rangle, \ |\uparrow\rangle, \ |\downarrow\rangle, \ |\uparrow\downarrow\rangle$

decoupling

$$S_i^+ S_j^- \ = \ c_{i\uparrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\uparrow} \ \approx < c_{i\uparrow}^\dagger c_{j\uparrow} > c_{i\downarrow} c_{j\downarrow}^\dagger - < c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger > c_{i\downarrow} c_{j\uparrow} + \dots$$

molecular fields

hopping-amplitude: $\xi_{i-j} \ = < c_{i\uparrow}^\dagger c_{j\uparrow} >$

pair-amplitude: $\Delta_{i-j} \ = < c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger >$

ground-state wavefunction

BCS-wavefunction

$$|\Psi_0\rangle \ = \ \prod_k \left(u_k + v_k c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger \right) |0\rangle$$

strong-coupling approach via RMFT

Hubbard Hamiltonian

canonical transformation $e^{iS}He^{-iS}$ $\Updownarrow$

t-J Hamiltonian

Gutzwiller renormalization g $\Downarrow$

renormalized Hamiltonian

mean-field decoupling ξ, Δ $\Downarrow$

renormalized mean-field Hamiltonian

ground state $|\Psi_0\rangle$ $\Downarrow$

trial projected wavefunction $|\Psi\rangle = P|\Psi_0\rangle$

Variational Monte Carlo

numerical evaluation

$$\frac{\langle\Psi|H_{t-J}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Psi_0|PH_{t-J}P|\Psi_0\rangle}{\langle\Psi_0|PP|\Psi_0\rangle}$$

[Zhang, Gros, Rice & Shiba '88]

order-parameter renormalization

order-parameter renormalization

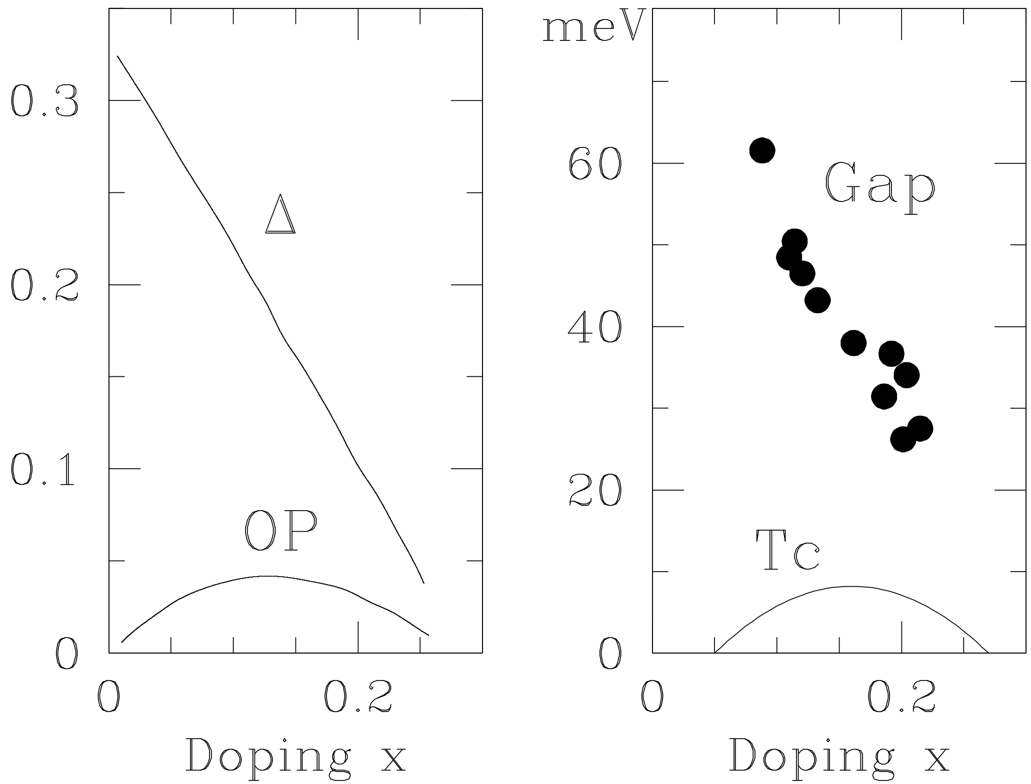
$$<c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}>_\psi \;=\; g_t \;<c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}>_{\psi_0}$$

$$\boxed{<\Delta>_\psi \;=\; g_t \;<\Delta>_{\psi_0}}$$

- Hubbard-U suppresses particle-number fluctuations

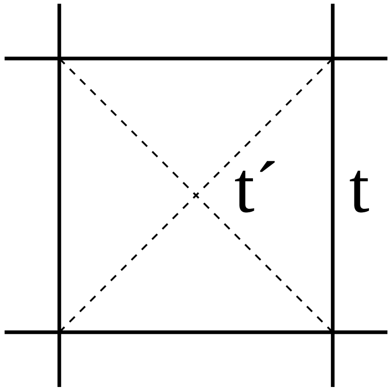
$$g_t \;=\; \frac{1-n}{1-n/2}$$

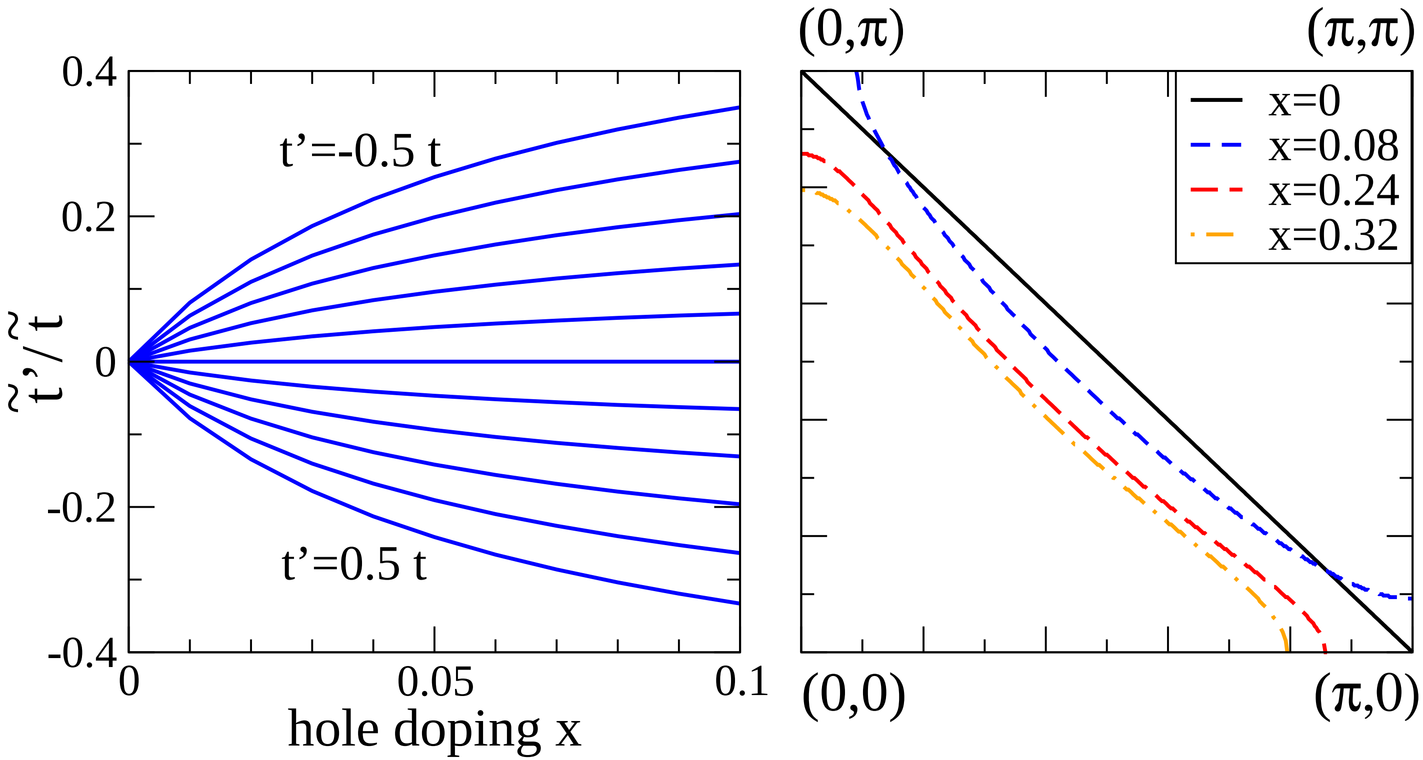
[Anderson *et al.* ‘04]



renormalization towards perfect nesting

RMFT $\lim_{n\to 1} \begin{cases} \tilde{t} = (t)_{\text{renorm}} & \to & J \\ \tilde{t}' = (t')_{\text{renorm}} & \to & 0 \end{cases}$





$t' = -t/4,\ U = 12t$

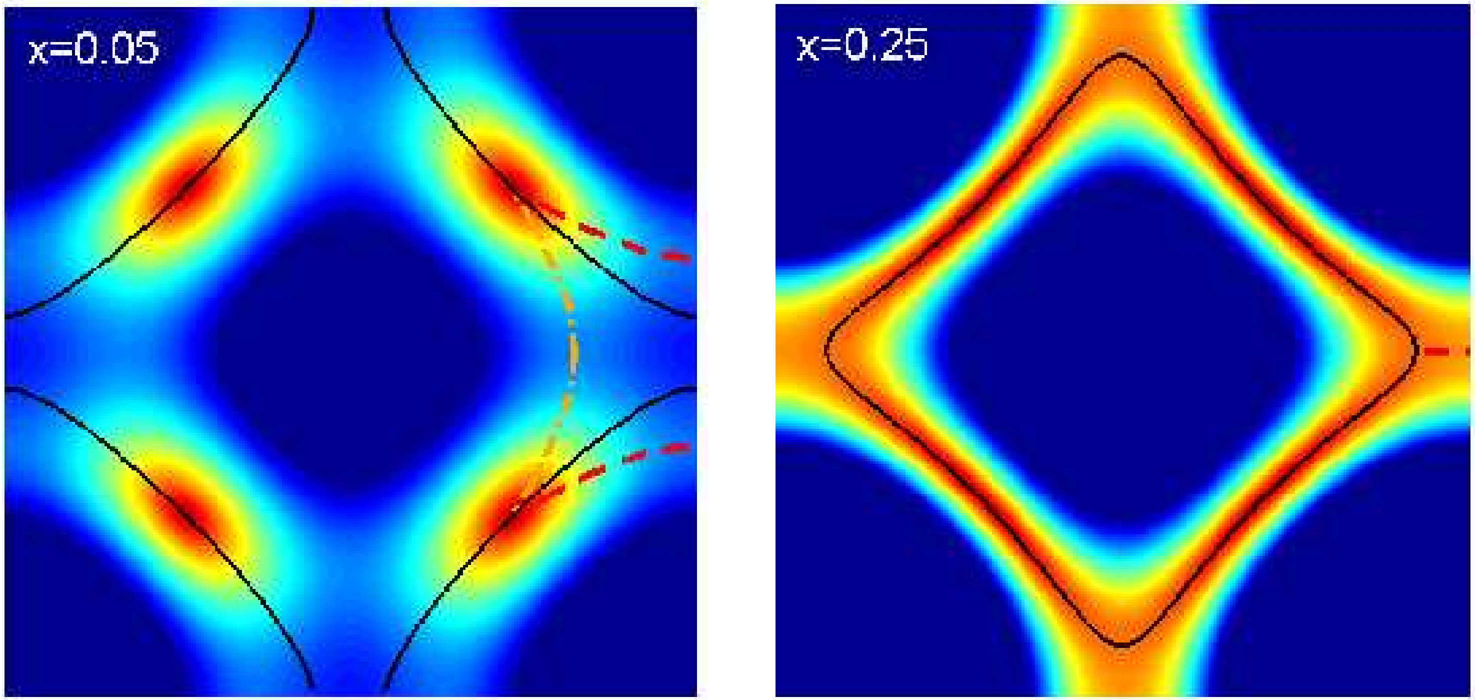
[Gros, Edegger, Muthukumar & Anderson, PNAS '06]

Fermi surface determination

large, momentum dependent gap Δ_k

'underlying Fermi surface' $\hat{=}$ Luttinger surface

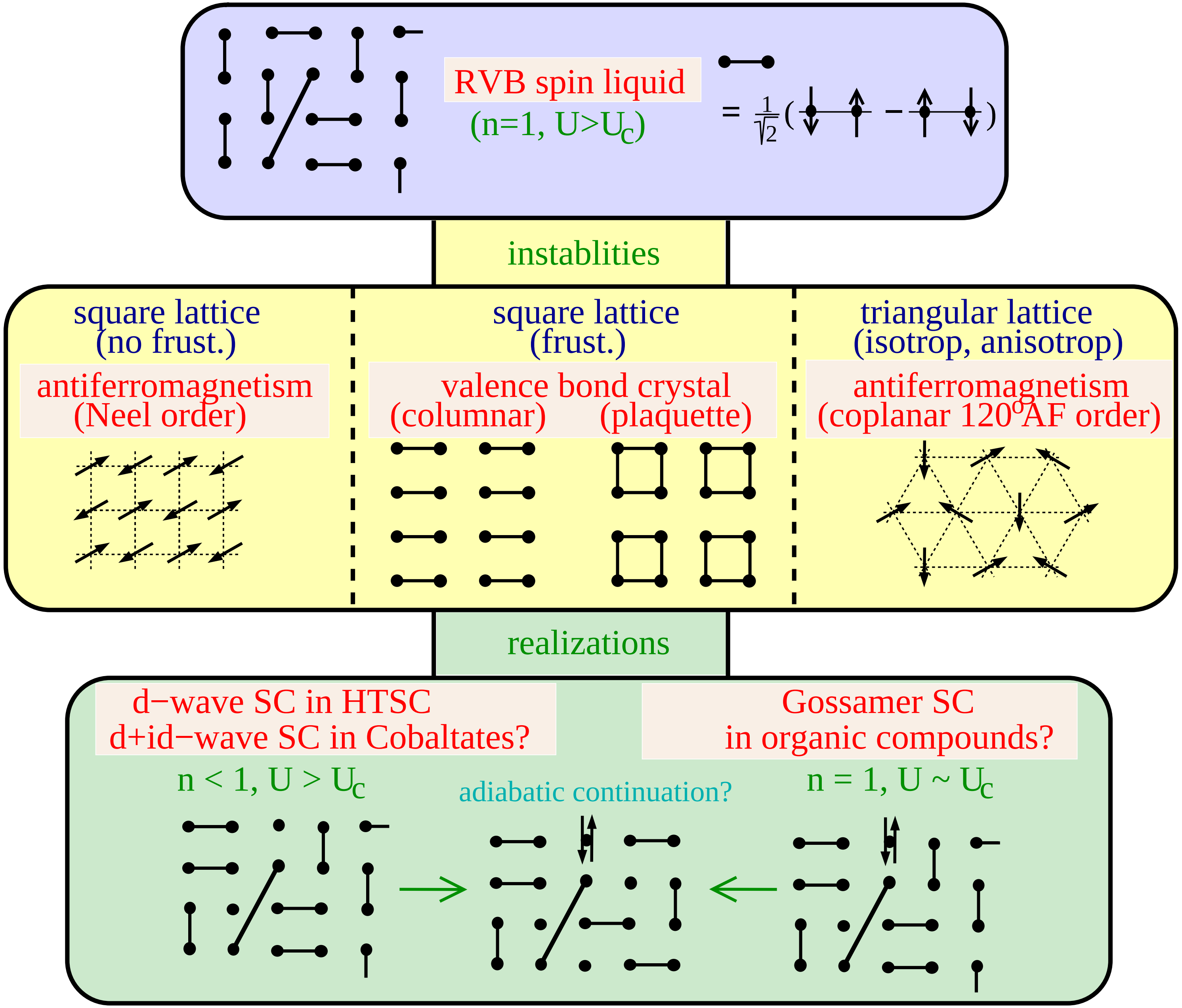
- $Re G(k, \omega)$ changes sign



intensity plots
line $\equiv$ Luttinger surf.

[Gros, Edegger, Muthukumar & Anderson, PNAS '06]

RVB as an unstable fixpoint

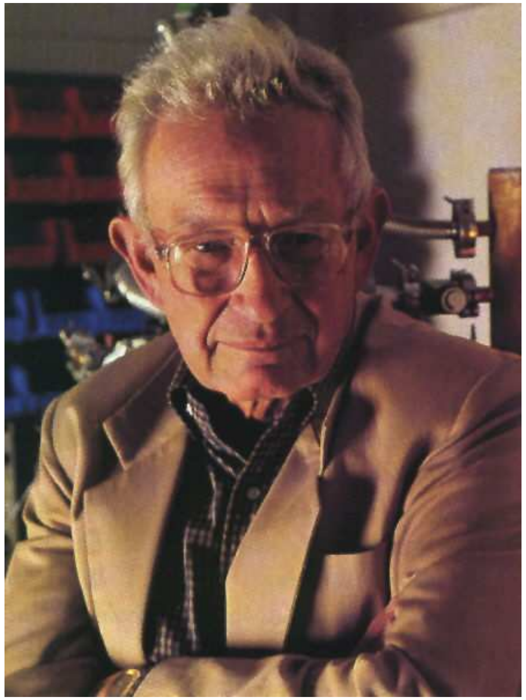


outlook

It's all fun together with ...

Bernhard Edegger

V.N. Muthukumar



P.W. Anderson

[PRL '06, PNAS '06, review on RVB-Gutzwiller '07]

variational Monte Carlo (VMC)

fixed particle number

$$|\Psi_0^N\rangle = P_N \prod_k \left(u_k + v_k c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger\right)|0\rangle = \text{const.} \times \Bigg(\underbrace{\sum_{r,r'} a(r-r') c_{r\uparrow}^\dagger c_{r'\downarrow}^\dagger}_{\text{pair wavefunction}} \Bigg)^{N/2} |0\rangle$$

$$a(\delta r) = \sum_k \frac{v_k}{u_k} \mathrm{e}^{ik\delta r}$$

matrix elements

$$\frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_{\alpha,\beta} \langle\alpha|\hat{O}|\beta\rangle \frac{\langle\Psi|\alpha\rangle\langle\beta|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_\alpha \left(\sum_\beta \frac{\langle\alpha|\hat{O}|\beta\rangle\langle\beta|\psi\rangle}{\langle\alpha|\psi\rangle}\right) \frac{|\langle\alpha|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle} \equiv \sum_\alpha f(\alpha)\rho(\alpha)$$

Monte Carlo walk

weight: $\rho(\alpha)$

method: update of inverse determinants $\langle\alpha|\Psi\rangle$

canonical transformation

kinetic energy terms

$$T = T_e + T_d + T_+ + T_-$$

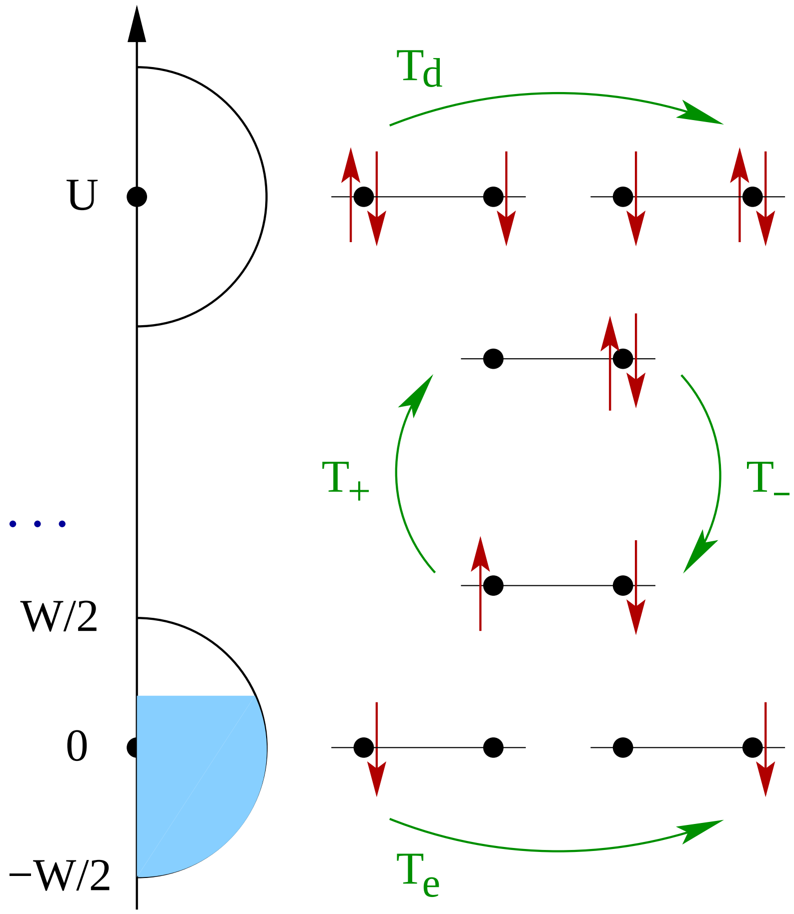
$$H = \left(T_e + T_d + U\sum_i n_{i,\uparrow}n_{i,\downarrow}\right) + \left(T_+ + T_-\right)$$

perturbation expansion

$$H_{eff} = e^{iS}He^{-iS} \approx H + i[S,H] + \frac{i^2}{2}[S,[S,H]] + \ldots$$

diagonal in double occupancy $\Rightarrow$

$$S = \frac{i}{U}\left(T_+ - T_-\right) + O(t^2/U^2)$$



projected Hilbert-space

$$H_{t-J} = H_{eff} + O(t^3/U^2) = T_e + T_d + U\sum_i n_{i,\uparrow}n_{i,\downarrow} + J\sum_{<i,j>}\mathbf{S}_i \cdot \mathbf{S}_j$$

$J = 4t^2/U$

Gutzwiller renormalization factors

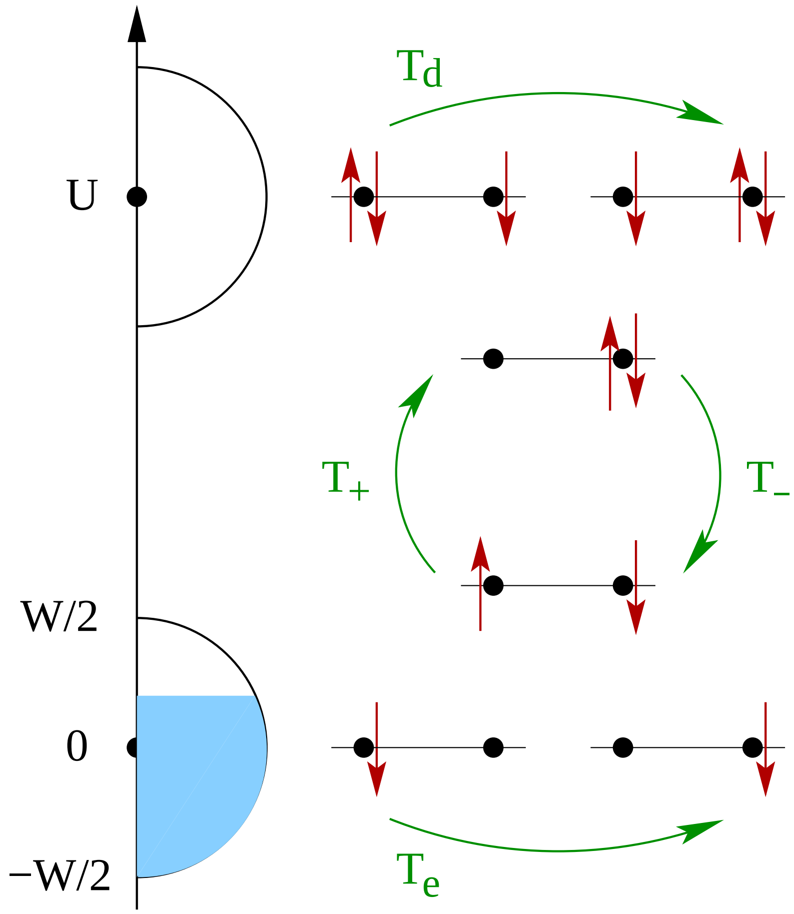
kinetic energy

$$\frac{\langle\Psi|T_e|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Psi|T|\Psi\rangle}{\langle\Psi|\Psi\rangle} \propto n_\sigma(1-n)$$

$$\frac{\langle\Psi_0|T|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \propto n_\sigma(1-n_\sigma)$$

$$\frac{\langle\Psi|T|\Psi\rangle}{\langle\Psi|\Psi\rangle} \approx g_t \frac{\langle\Psi_0|T|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

$$g_t = \frac{1-n}{1-n_\sigma} = \frac{1-n}{1-n/2}$$



renormalized Hamiltonian

in pre-projected Hilbert space

d-wave superconductivity (RMFT)

$$|\Psi_0\rangle = \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{k\downarrow}\right)|0\rangle \qquad u_k^2/v_k^2 = \frac{1}{2}\left(1 \pm \frac{\tilde{\varepsilon}_k}{\sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}}\right)$$

parameterization

$$\tilde{\varepsilon}_k = \left(-2g_t t + \tfrac{3}{4} g_s J \xi\right)\left(\cos k_x + \cos k_y\right)$$
$$\Delta_k = \tfrac{3}{4} g_s J \Delta \left(\cos k_x - \cos k_y\right)$$

$x \leftrightarrow y$ d-wave symmetry

results

- predicted d-wave superconductivity

[Gros '88]

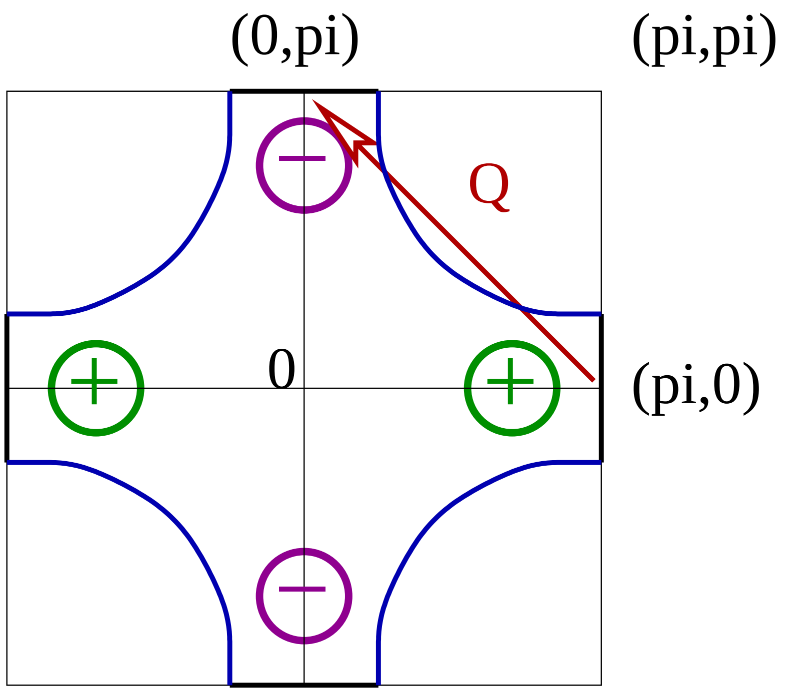
- contains pseudogap

[Zhang, Gros, Rice & Shiba '88]

Why two dimensions?

antiferromagnetic nesting vector

- 3 dimensions $\mathbf{Q} = (\pi, \pi, \pi)$
- 2 dimensions $\mathbf{Q} = (\pi, \pi)$



BCS gap-equation

$$\Delta_{\mathbf{k}} = -\int \frac{d^2 p}{(2\pi)^2} V_{\mathbf{k}-\mathbf{p}} \frac{\Delta_{\mathbf{p}}}{\sqrt{\xi_{\mathbf{p}}^2 + \Delta_{\mathbf{p}}^2}}$$

repulsive interaction

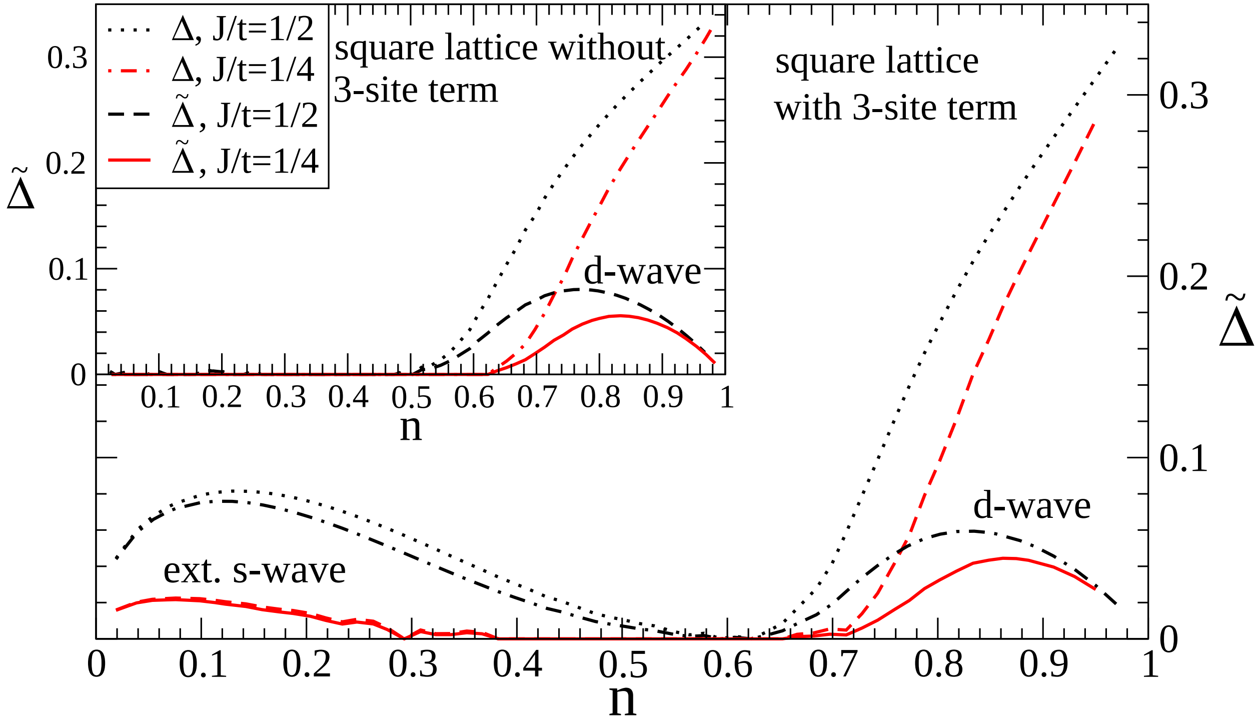
- $\boxed{V_{\mathbf{k}-\mathbf{p}} \propto J > 0}$
- scattering between hot-spots $(\pi, 0)$ and $(0, \pi)$ via $\mathbf{Q} = (\pi, \pi)$
  - ▷ d-wave: $\boxed{\Delta_{(\pi,0)} = -\Delta_{(0,\pi)}}$

phase diagram

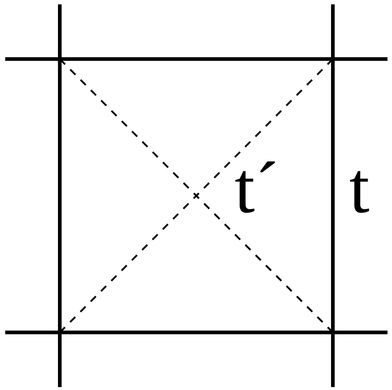
2D t-J model

$$H_{t-J} = \sum_{<i,j>,\sigma} t_{(i,j)} \left(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right) + \sum_{<i,j>} \frac{4t^2_{(i,j)}}{U} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right)$$
$$- \sum_{\sigma,\sigma'} \sum_{<i,j>,<j,l>} \frac{t_{(i,j)} t_{(j,l)}}{U} \left(c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{j\sigma'} c_{l\sigma'} + k.k. \right)$$

[Edegger, Gros, Muthukumar '05]



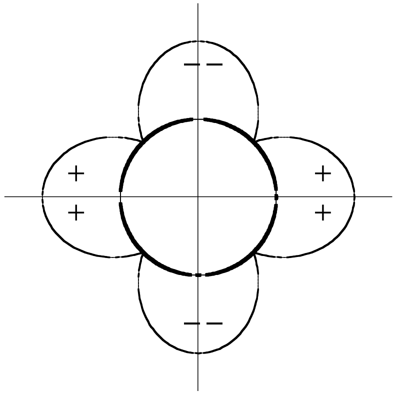
HTSC: $t_2/t_1 \approx 1/3$

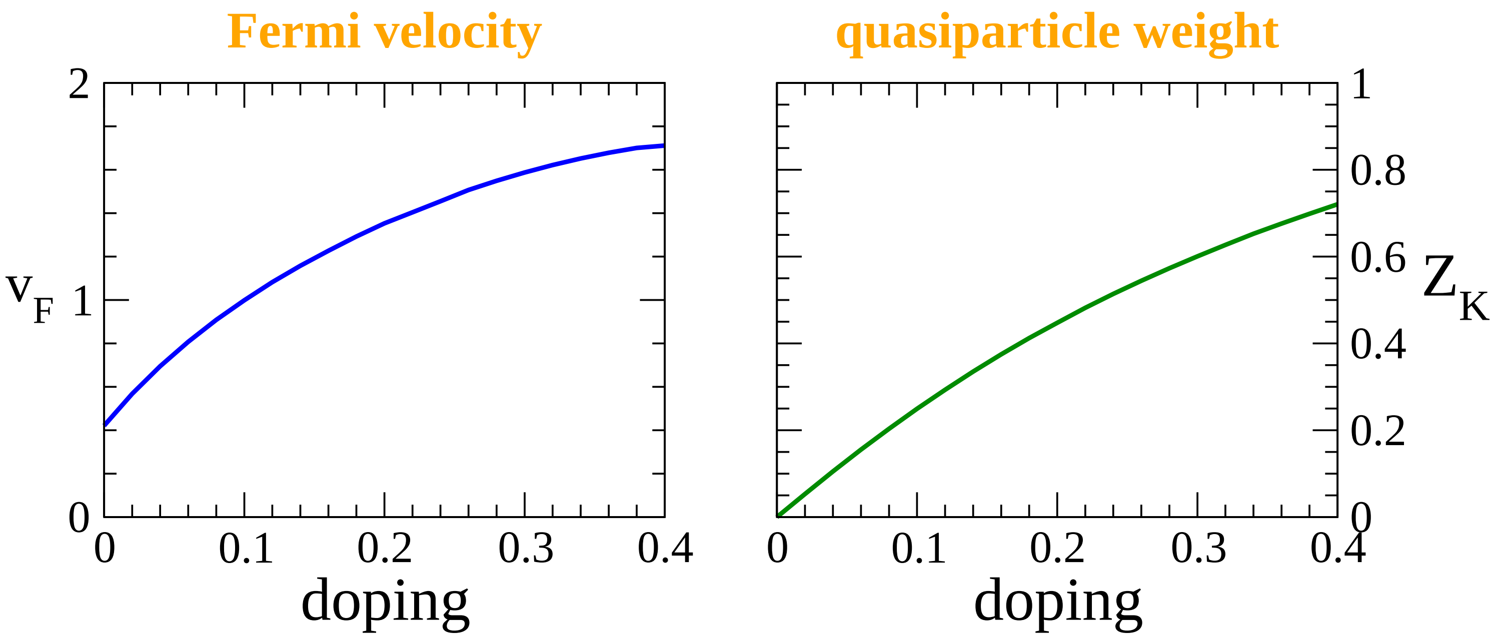


nodal quasiparticles

d-wave superconductor

- no gap along $(1,1)$
  - ▷ renormalized mean-field theory for the HTSC





[Edegger, Muthukumar, Gros, Anderson '06]

Theories for HTSC

microscopic approaches

- strong coupling: RMFT and projected wavefunctions
  [Anderson, Lee, Zhang, Trivedi, Gros, ...]
- weak coupling: spin fluctuations
  [Pines, ...]
- phonons: favor s-wave
  [Müller, Shen, ...]

phenomenological approaches

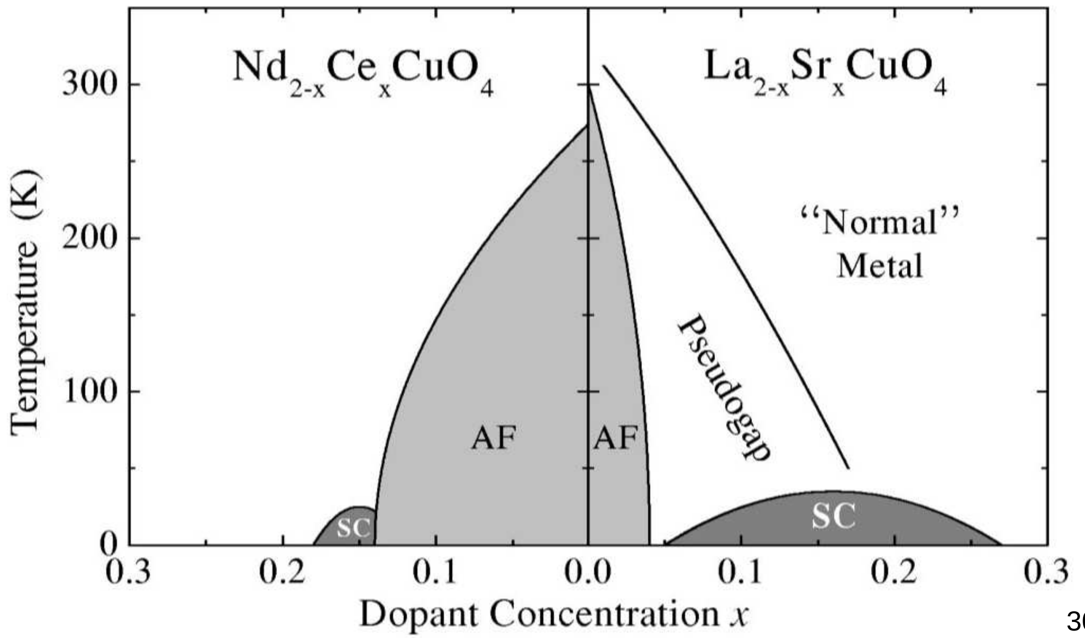
- SU(5): between SC and AF order parameter
  [Zhang, Hanke, ...]
- stripes: charge vs. spin ordering, 1/8-doping
  [Kivelson, Zaanen, ...]
- marginal Fermi liquid: scattering rate in normal state $\propto |\omega|$
  [Varma, ...]

physics of HTSC within RVB/RMFT

correlations

- induce antiferromagnetism — at half-filling
- induce superconductivity — at finite doping
- suppress particle-number fluctuations — close to half-filling
  - ▷ suppress long-range superconductivity — close to half-filling
  - ▷ lead to the pseudogap phase — close to half-filling

$$T_c \propto (1-n)J$$



applications and generalizations

high-temperature superconductors

- phase-diagram, quasi-particles, ARPES, ...
  [Randeria, Trivedi, Dagotto, Sorella, Lee, Ivanov, ...]
- stripes and dynamics
  [Seibold, Lorenzana, ...]
- 'Gossamer superconductivity'
  [Laughlin, ...]

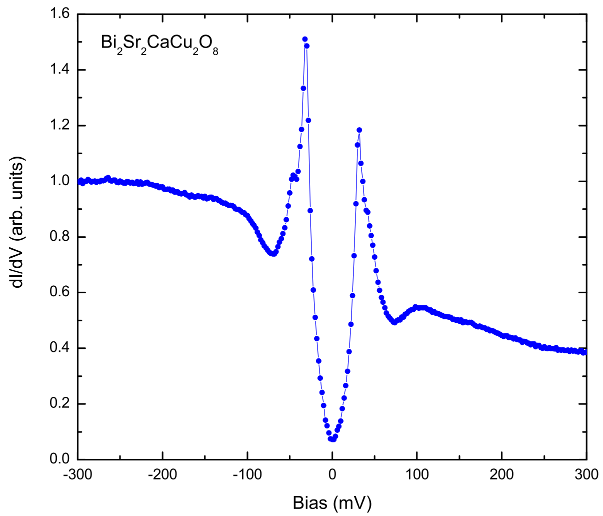
other correlated systems

- cobalt and organic superconductors
  [McKenzie, Zhang, Baskaran, Trivedi, Ogata, Schmalian ...]
- frustrated magnets
  [Mila, Giamarchi, ...]
- multi-orbitals and magnetism in Fe, Ni
  [Weber, Gebhard, Bünemann, ...]

partially projected wavefunctions

$$|\Psi'_l\rangle = P'_l\,|\Psi_0\rangle, \qquad P'_l = \prod_{i\neq l}(1-n_{i\uparrow}n_{i\downarrow})$$

- no double occupancy except the site l (reservoir site)
- Motivation: excited states, e.g. $|\Psi^+_{k\sigma}\rangle = Pc^\dagger_{k\sigma}|\Psi_0\rangle$
  - ▷ calculation of matrix elements, e.g. $\langle\Psi|c_{k\sigma}|\Psi^+_{k\sigma}\rangle = \langle\Psi|Pc_{k\sigma}Pc^\dagger_{k\sigma}|\Psi_0\rangle$
  - ▷ commutations of projection operators with creation/destruction operators: $Pc_{l\uparrow} = c_{l\uparrow}P'_l \;\Rightarrow$ $\dfrac{\langle\Psi'_l|\hat{O}|\Psi'_l\rangle}{\langle\Psi'_l|\Psi'_l\rangle} = g'\,\dfrac{\langle\Psi_0|\hat{O}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$



Asymmetry in tunnelling matrix elements?

[Anderson & Ong '04]

Can we explain it within RMFT?

Occupancy of the reservoir site (1)

- We define:

$$X = \frac{\langle\Psi_0|PP|\Psi_0\rangle}{\langle\Psi_0|P_l'P_l'|\Psi_0\rangle} = \frac{\langle\Psi|\Psi\rangle}{\langle\Psi_l'|\Psi_l'\rangle}$$

- Gutzwiller approximation
(considering the relative sizes of the Hilbert spaces):

$$X \sim \frac{\frac{L!}{N_\uparrow!N_\downarrow!N_h!}}{\frac{L!}{N_\uparrow!N_\downarrow!N_h!} + \frac{(L-1)!}{(N_\uparrow-1)!(N_\downarrow-1)!(N_h+1)!}},$$

where $L = N_\uparrow + N_\downarrow + N_h$.

$$\Rightarrow \quad X \approx \frac{1-n}{(1-n_\uparrow)(1-n_\downarrow)}$$

Occupancy of the reservoir site (2)

- Exact relations for the reservoir site

$$
\begin{aligned}
\langle (1-n_{l\uparrow})(1-n_{l\downarrow})\rangle_{\Psi'_l} &= X\,(1-n) \\
\langle n_{l\sigma}(1-n_{l-\sigma})\rangle_{\Psi'_l} &= X\,n_\sigma \\
\langle d\rangle_{\Psi'_l} = \langle n_{l\uparrow}n_{l\downarrow}\rangle_{\Psi'_l} &= 1-X
\end{aligned}
$$

- Proof for first equation: Since, $n_l = n_{l,\uparrow} + n_{l,\downarrow}$ and

$$\langle \Psi_0|P(1-n_l)P|\Psi_0\rangle = \langle \Psi_0|P'_l(1-n_{l\uparrow})(1-n_{l\downarrow})P'_l|\Psi_0\rangle$$

we have,

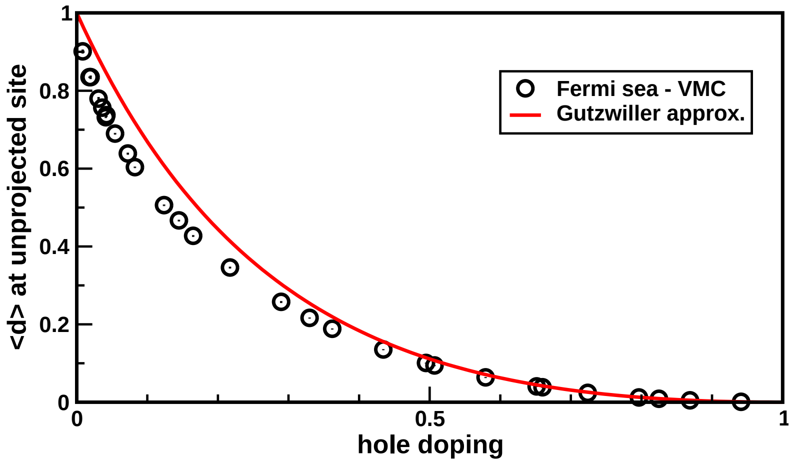
$$\langle (1-n_{l\uparrow})(1-n_{l\downarrow})\rangle_{\Psi'_l} = \frac{\langle \Psi|(1-n_l)|\Psi\rangle}{\langle \Psi|\Psi\rangle}\,\frac{\langle \Psi|\Psi\rangle}{\langle \Psi'_l|\Psi'_l\rangle} = (1-n)X.$$

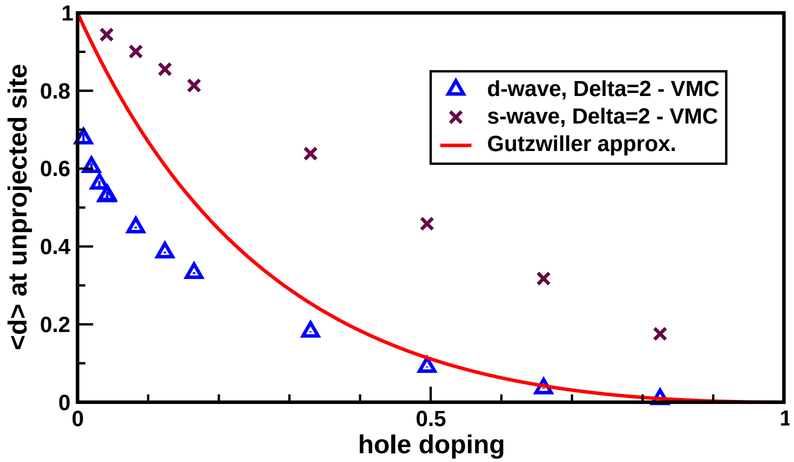
Variational Monte Carlo

double occupancy of the reservoir site

$$\langle d \rangle_{\Psi'_l} = 1 - X$$

as a function of doping by VMC





Good agreement
for Fermi sea!

Clear deviations
from Gutzwiller approximation for BCS wavefunction!

Tunneling Matrix Elements

particle excitation

$$|\Psi^{+}_{k\sigma}\rangle = P c^{\dagger}_{k\sigma}|\Psi_0\rangle$$
$$N^{+}_{k\sigma}/N_G = g_{t,\sigma}\left(1 - n^{0}_{k\sigma}\right)$$

hole excitation

$$|\Psi^{-}_{k\sigma}\rangle = P c_{k\sigma}|\Psi_0\rangle$$
$$N^{-}_{k,\sigma}/N_G = n_{k\sigma}/g_{t,-\sigma}$$

$$N^{\pm}_{k,\sigma} = \langle\Psi^{\pm}_{k\sigma}|\Psi^{\pm}_{k\sigma}\rangle; \qquad N_G = \langle\Psi|\Psi\rangle; \qquad n^{0}_{k\sigma} = \langle c^{\dagger}_{k\sigma}c_{k\sigma}\rangle_{\Psi_0};$$

tunneling matrix elements = quasiparticle renormalization

$$M^{+}_{k\sigma} = \frac{\left|\langle\Psi^{+}_{k\sigma}|c^{\dagger}_{k\sigma}|\Psi\rangle\right|^{2}}{N^{+}_{k\sigma}N_G} = g_{t,\sigma}(1 - n^{0}_{k\sigma})$$

$$M^{-}_{k\sigma} = \frac{\left|\langle\Psi^{-}_{k\sigma}|c_{k\sigma}|\Psi\rangle\right|^{2}}{N^{-}_{k\sigma}N_G} = g_{t,-\sigma}n^{0}_{k\sigma}$$

$\Rightarrow$ Matrix elements vanish at half-filling for $n \to 1$

$$g_t = \frac{1-n}{1-n/2} \to 0$$

Hole excitation (1)

normalization of hole excitation

$$N^{-}_{k\sigma}/N_G = \langle\Psi^{-}_{k\sigma}|\Psi^{-}_{k\sigma}\rangle/N_G = \frac{1}{N_G L}\sum_{l,m} \mathrm{e}^{ik(l-m)}\langle\Psi_0|P'_l c^{\dagger}_{l\sigma}c_{m\sigma}P'_m|\Psi_0\rangle$$

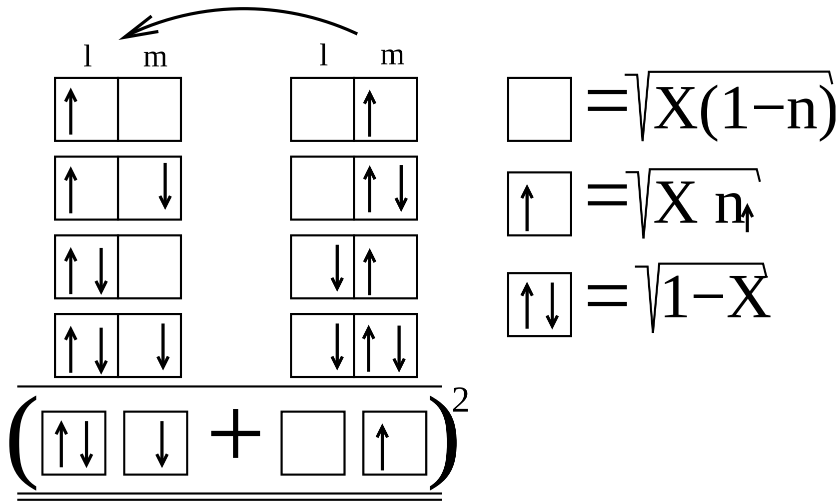
$$= \frac{1}{X}\left[Xn_\sigma + (1-X)\right] + \frac{1}{N_G L}\sum_{l\neq m} \mathrm{e}^{ik(l-m)}\langle\Psi_0|P'_{lm} c^{\dagger}_{l\sigma}c_{m\sigma}P'_{lm}|\Psi_0\rangle$$

the off-site term

$$\langle\Psi_0|P'_{lm} c^{\dagger}_{l\sigma}c_{m\sigma}P'_{lm}|\Psi_0\rangle/N_G$$

$$= \frac{\langle\Psi_0|P'_{lm}P'_{lm}|\Psi_0\rangle}{\langle\Psi_0|P\,P|\Psi_0\rangle}\,\frac{\langle\Psi_0|P'_{lm}c^{\dagger}_{l\sigma}c_{m\sigma}|\Psi_0\rangle}{\langle\Psi_0|P'_{lm}P'_{lm}|\Psi_0\rangle}$$

$$= \frac{1}{X^2}\,\frac{\left[\sqrt{X(1-n)}\sqrt{Xn_\sigma} + \sqrt{Xn_{-\sigma}}\sqrt{1-X}\right]^2}{n_\sigma(1-n_\sigma)}$$



$\Rightarrow$ insert Gutzwiller result for X:

$$\frac{N^{-}_{k,\sigma}}{N_G} = n^0_{k\sigma}\frac{1-n_{-\sigma}}{(1-n)} = \frac{n^0_{k\sigma}}{g_{t,-\sigma}}$$

Hole excitation (2)

matrix elements

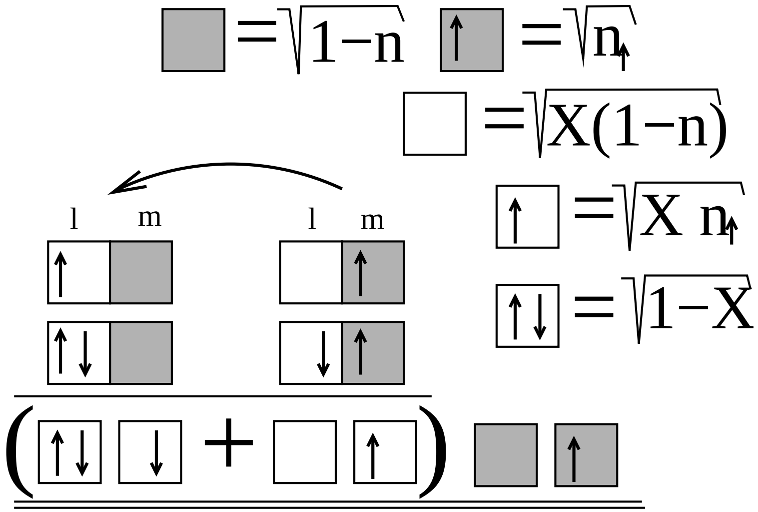
$$\frac{\langle\Psi_0|c^\dagger_{k\sigma}Pc_{k\sigma}P|\Psi_0\rangle}{N_G} = \frac{1}{N_GL}\sum_{l,m}\mathrm{e}^{ik(l-m)}\langle\Psi_0|P'_lc^\dagger_{l\sigma}c_{m\sigma}P|\Psi_0\rangle = \frac{Xn_\sigma}{X} + \frac{1}{N_GL}\sum_{l\neq m}\mathrm{e}^{ik(l-m)}\langle\Psi_0|P'_lc^\dagger_{l\sigma}c_{m\sigma}P'_l|\Psi_0\rangle$$

off-diagonal term

$$\frac{1}{N_G}\langle\Psi_0|P'_lc^\dagger_{l\sigma}c_{m\sigma}P'_l|\Psi_0\rangle$$

$$=\frac{\Psi_0|P'_lP'_l|\Psi_0\rangle}{N_G}\,\frac{\langle\Psi_0|P'_lc^\dagger_{l\sigma}c_{m\sigma}P'_l|\Psi_0\rangle}{\Psi_0|P'_lP'_l|\Psi_0\rangle}$$

$$=\frac{1}{X}\,\frac{\left[\sqrt{Xn_{-\sigma}}\sqrt{1-X}+\sqrt{X(1-n)}\sqrt{Xn_\sigma}\right]\sqrt{1-n}\sqrt{n_\sigma}}{(1-n_\sigma)n_\sigma}$$



normalized hole tunneling matrix element

$$M^-_{k\sigma} = \frac{\left|\langle\Psi^-_{k\sigma}|c_{k\sigma}|\Psi\rangle\right|^2}{N^-_{k\sigma}N_G} = g_{t,-\sigma}n^0_{k\sigma}$$

Density oscillations near the reservoir site (1)

- Motivation
  Gutzwiller approximation exact, if all states in the Hilbert space contribute equally
  - ▷ corresponds to uniform density of holes

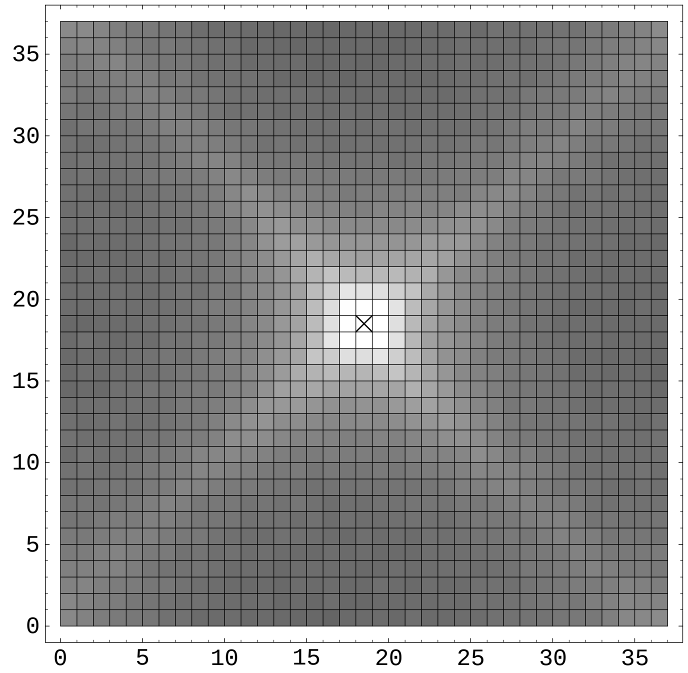
- we consider $|\Psi'_l\rangle$ at half-filling, $n_\uparrow = n_\downarrow = 1/2$, by VMC

- results for the hole density

$$n_h(i) \; = \; \langle 1 - n_i \rangle_{\Psi'_l}$$

are illustrated (holes in white)

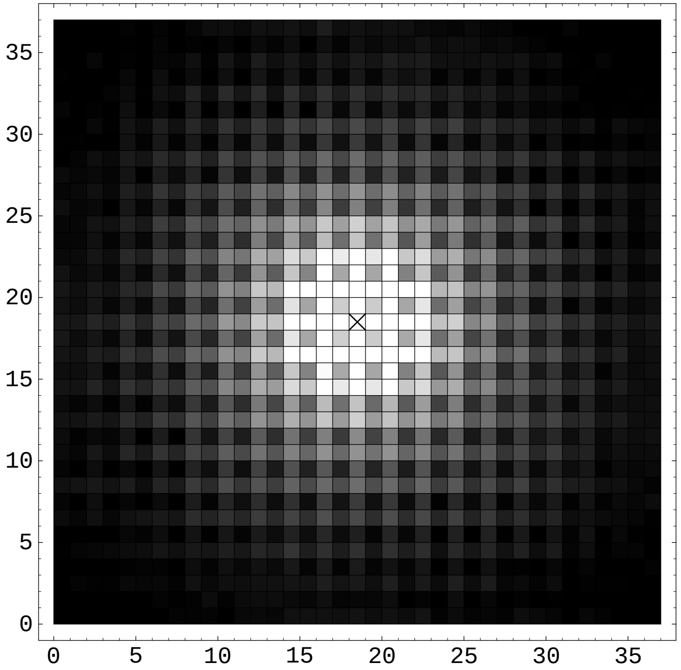
Projected Fermi Sea



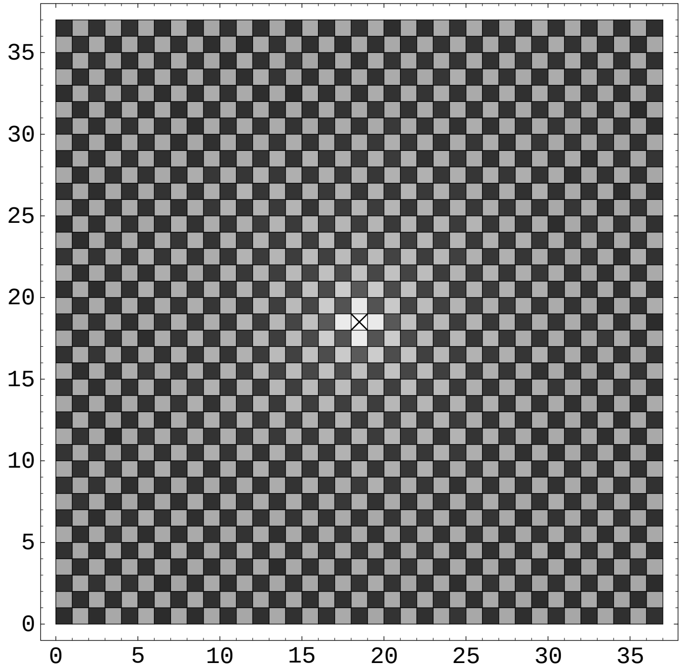
relative uniform distribution ⇒
good agreement with
Gutzwiller approx. reasonable

Density oscillations near the reservoir site (2)

Projected d-wave state



Projected s-wave state



quasi-checker-board pattern

checker-board pattern

$\Rightarrow$ no uniform distribution of holes

$\Rightarrow$ disagreements with Gutzwiller approx. reasonable

$\Rightarrow$ possible improvement by including off-site correlations

$\Rightarrow$ d-wave: similar patterns observed by STM in high-T_C-SC

Coherent and incoherent quasi-particles

$$
\begin{aligned}
c^{\dagger}_{k,\sigma}P_G|\Psi_0\rangle &= P_G\, c^{\dagger}_{k,\sigma}|\Psi_0\rangle + \frac{1}{\sqrt{L}}\sum_R e^{ikR}\, n_{R,-\sigma}c^{\dagger}_{R,\sigma}P_G|\Psi_0\rangle \approx P_G\, c^{\dagger}_{k,\sigma}|\Psi_0\rangle \\
c_{k,\sigma}P_G|\Psi_0\rangle &= P_G\, c_{k,\sigma}|\Psi_0\rangle - \frac{1}{\sqrt{L}}\sum_R e^{ikR}\, P_G n_{R,-\sigma}c_{R,\sigma}|\Psi_0\rangle
\end{aligned}
$$

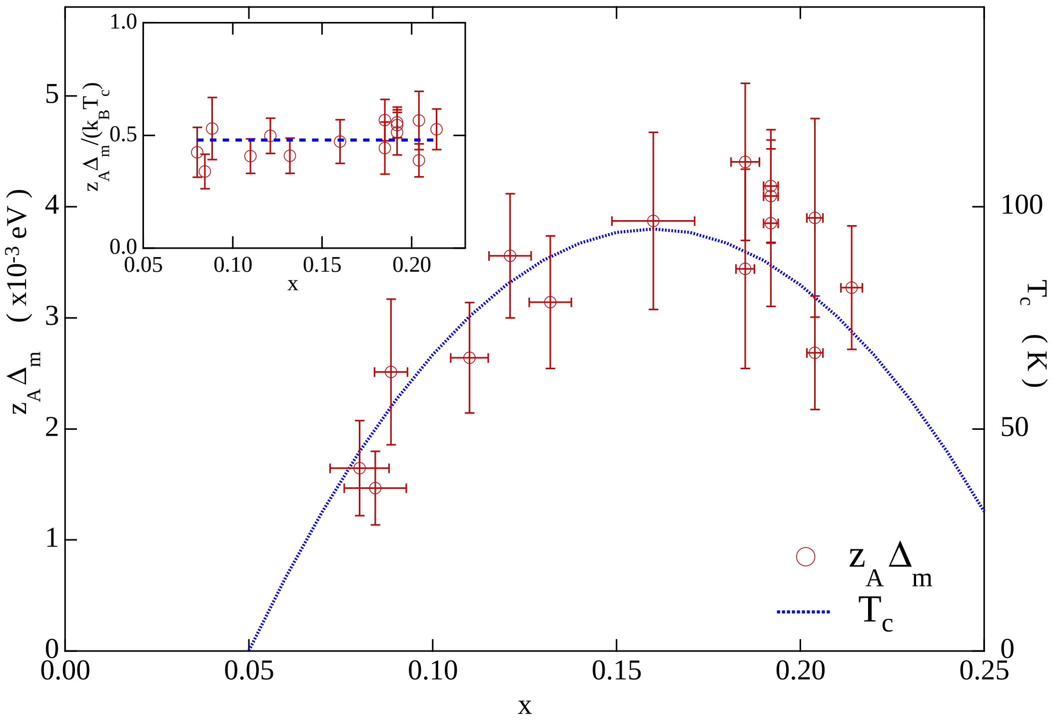
- No incoherent contribution to quasi-particle
- Incoherent contribution to quasi-hole $\rightarrow$ orthogonalization

$$
c^{\dagger}_{k,\sigma}|\Psi_0\rangle = |2\rangle + |3\rangle = \tilde{b}_2|\tilde{2}\rangle + \tilde{b}_3|\tilde{3}\rangle
$$

with $|\tilde{2}\rangle = \frac{|2\rangle}{\sqrt{\langle 2|2\rangle}}, \qquad |\tilde{3}\rangle = \frac{|3\rangle - |2\rangle\langle 2|3\rangle/\langle 2|2\rangle}{\sqrt{\langle 3|3\rangle - |\langle 2|3\rangle|^2/\langle 2|2\rangle}}, \qquad \langle\tilde{2}|\tilde{3}\rangle = 0$. and

$$
\boxed{\tilde{b}_2^2 = \frac{4xn^0_{k\sigma}}{2(1+x)}\ .} \qquad \boxed{\tilde{b}_3^2 = 1 - \tilde{b}_2^2\ .}
$$

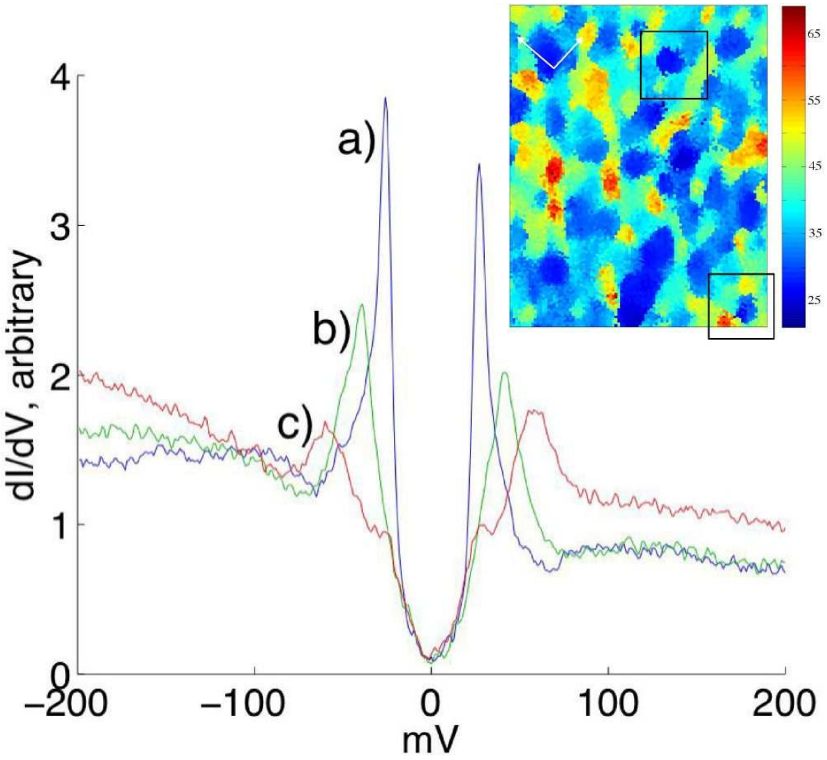
ARPES-experiment



“Coherent quasiparticle weight and its connection to high-Tc superconductivity from angle-resolved photoemission”
Ding, Engelbrecht, Wang, Campuzano, Wang, Yang, Rogan, Takahashi, Kadowaki, Hinks,

Phys. Rev. Lett. **87**, 227001 (2001)

Coherent and incoherent spectral weight



[Fang *et al.* '05]

- coherent part of quasiparticles symmetric at Fermi surface
  ▷ incoherent contribution

[Randeria et al. '04]

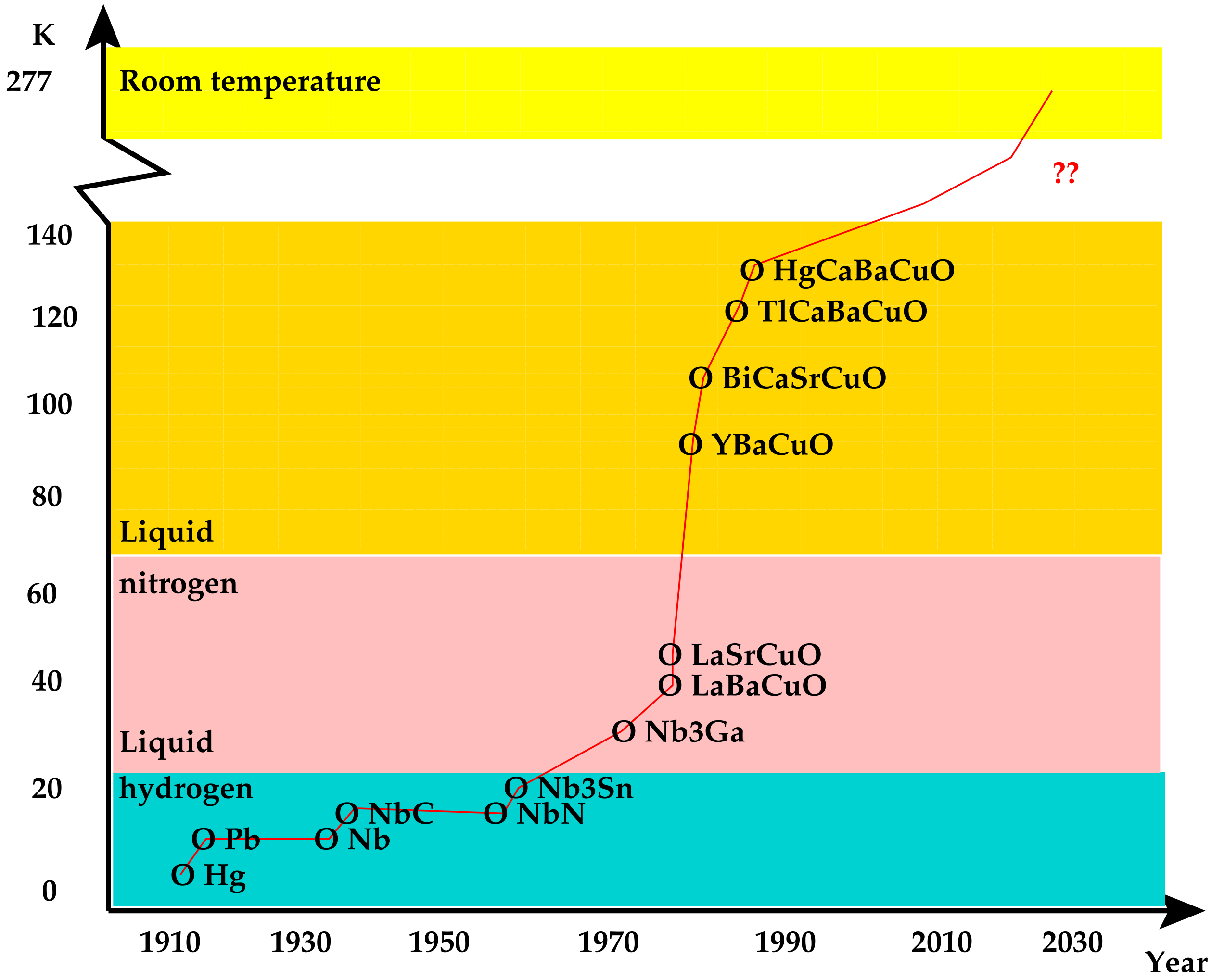
momentum distribution function

$$\frac{\langle\Psi|c^\dagger_{k\sigma}c_{k\sigma}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \equiv n_k = g_t\, n^0_k + \frac{(n/2)^2}{1-n/2} \qquad n^0_k = \frac{\langle\Psi_0|c^\dagger_{k\sigma}c_{k\sigma}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

$$g_t = \frac{1-n}{1-n/2} \equiv Z_k$$

quasi-particle renormalization weight

Transition temperatures



1986: Discovery by of high-temperature superconductivity by Bednorz & Müller